Covariance matrices for nuclear decay and fission yield data

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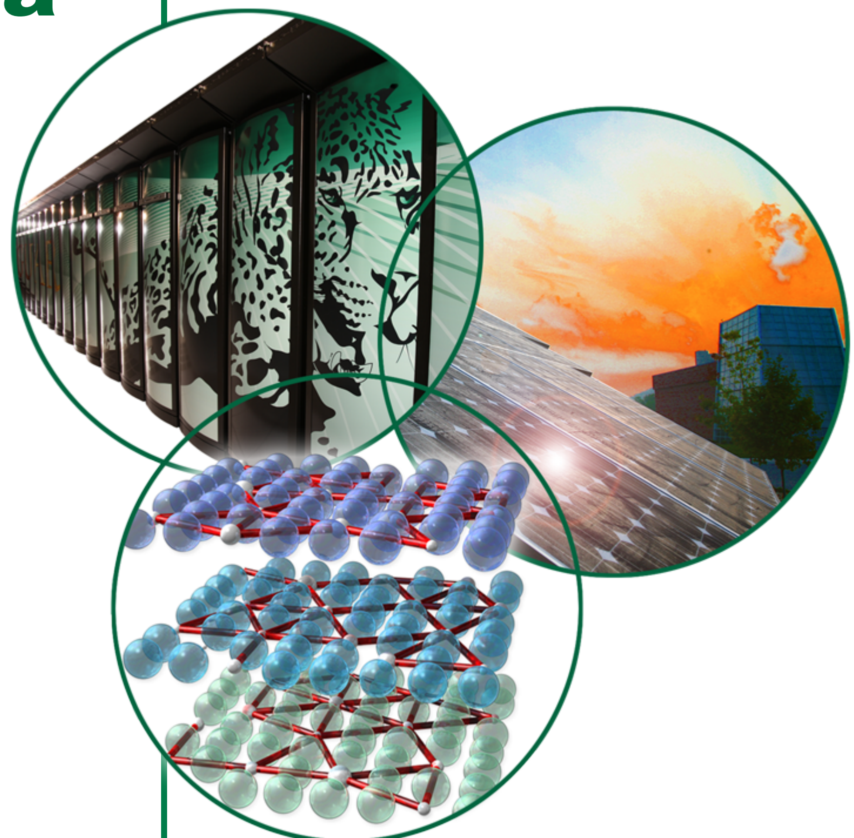


Overview of the project

Goal : develop methods to predict the uncertainties in used nuclear fuel properties due to the underlying uncertainties (and related correlations) in decay and fission yield data

ORNL already has capability to propagate cross-section uncertainties/ correlations. We want to use this capability for decay data and fission product yields.

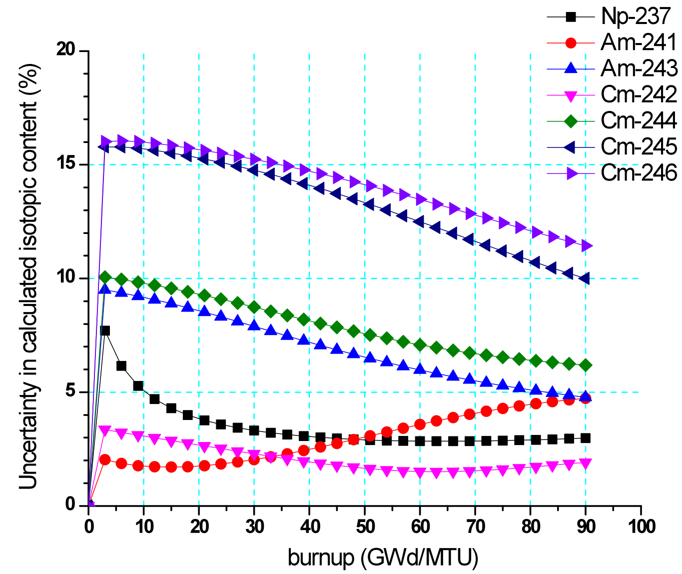
Step 1 : generate covariance library for nuclear decay and fission yield data (Williams/Gauld/Pigni)

- compile uncertainties for nuclear decay and fission yields data
- develop methods to generate related covariance matrices

Step 2 : Monte Carlo-based uncertainty methods developed for analysis of covariance matrices will be used to generate perturbed covariance libraries developed in Step 1 (Wiarda/Gauld/Pigni)

Applications : demonstrate the feasibility of the project on applications, i.e. fuel decay heat, radio toxicity, burn up credit analysis

Isotope	Number of measured samples	Uncertainty in calculated isotopic content using radiochemical assay data (%)	Uncertainty in calculated isotopic content due to cross section data uncertainties (%)
^{235}U	92	3.5	1.2
^{236}U	77	3.5	1.4
^{238}U	92	0.4	<0.1
^{238}Pu	77	5.9	4.3
^{239}Pu	92	3.5	1.5
^{240}Pu	92	3.4	1.9
^{241}Pu	92	4.5	1.6
^{242}Pu	91	6.1	2.6
^{244}Cm	57	11.1	8.4
^{245}Cm	24	15.6	14.2
^{246}Cm	14	25.5	14.8
^{90}Sr	15	6.9	0.2
^{133}Cs	10	1.7	0.7
^{134}Cs	59	7.1	4.3
^{135}Cs	16	3.7	3.0
^{137}Cs	73	3.1	<0.1
^{143}Nd	36	3.2	1.2
^{145}Nd	36	2.2	1.2
^{148}Nd	77	1.4	0.4
^{144}Ce	32	8.1	0.1
^{147}Sm	24	3.4	1.5
^{149}Sm	20	6.2	4.1
^{150}Sm	24	3.2	2.8
^{151}Sm	24	4.4	0.2
^{152}Sm	24	3.7	0.1
^{151}Eu	12	19.8	3.6
^{153}Eu	19	3.1	2.2
^{154}Eu	44	10.4	7.1
^{155}Eu	11	7.7	5.2
^{155}Gd	19	14.4	5.0



- Isotopic uncertainties based on Monte Carlo sampling of cross section covariance data

Key points and assumptions for step 1

Compile available uncertainties:

In ENDF/B-VII.1 library uncertainties of cumulative and independent yields as well as of half-lives and energies are already present

No new evaluations:

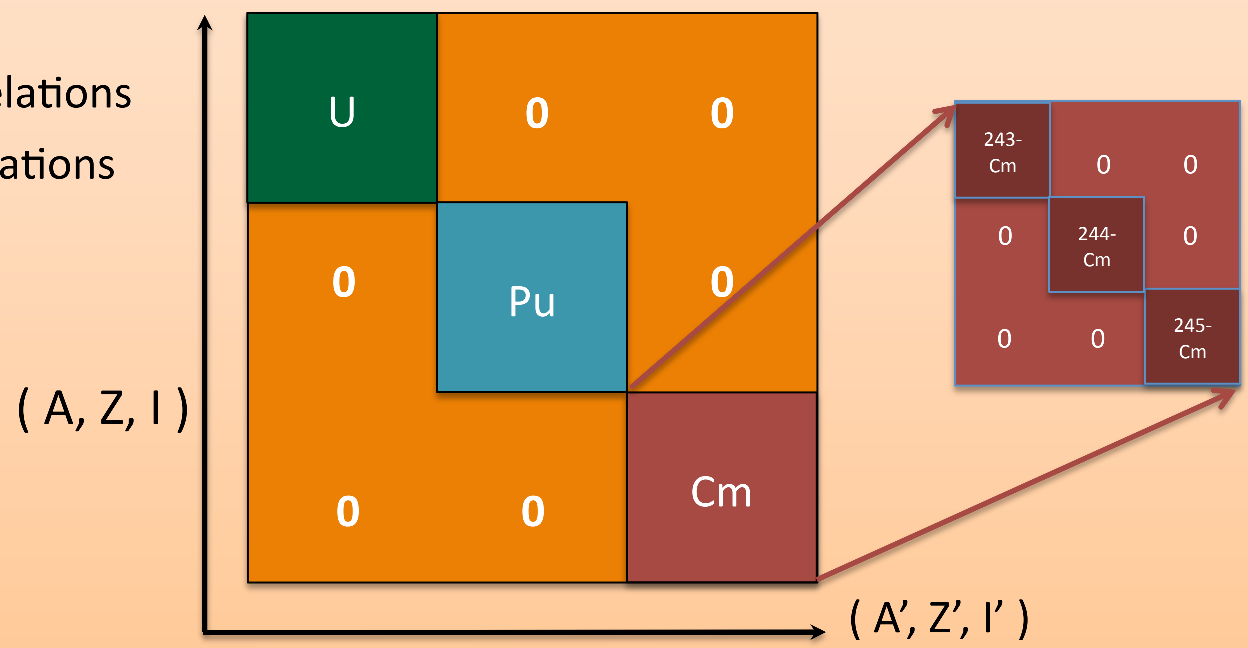
We only want to generate covariance matrices, e.g. of fission independent/cumulative yields, with no intent to re-evaluate ENDF/B-VII.1 yield library

Initial assumptions to generate correlations for fission product yields:

-No energy dependence

-No cross-material correlations

-No cross-isotope correlations



Some work on FPY and decay evaluations

1991 – The UK Fission Product Library Version 2 (UKFY2)
M.F. James, R.W. Mills and *D.R. Weaver*

1994 – Sensitivity and Uncertainty Analysis for Fission Product Decay heat Calculations
J. Rebah, Y.K. Lee, J.C. Nimal et al.

2010 – Fission Product Yields from Fission Spectrum n+^{239}Pu for ENDF/B-VII.1
M.B. Chadwick, T. Kawano, D.W. Barr et al.

2011 – JENDL FP Decay Data File 2011 and Fission Yields Data File 2011
Jun-ichi Katakura

Present – WPEC subgroup 37 – Improved fission product yield evaluation methodologies – Co-ordinator: R. W. Mills

Definitions and constraints

Independent fission yield from the fission of a nucleus with mass number A_T and atomic number Z_f :

$$y \equiv y(A,Z,I;\vec{x}) \quad \text{where} \quad \vec{x} \equiv \vec{x}(A_f, Z_f, E)$$

For neutron-induced fission, $A_f = A_T + 1$

For spontaneous fission, $A_f = A_T$

Generally, for a semi-empirical model, the independent fission yield depends on a set of parameters:

$$\vec{x} = \{\vec{\mu}(A_f, Z_f, E), \vec{\lambda}(A_f, Z_f, E)\}$$

Constraints

$$\sum_Z f(A,Z;\lambda) = 1 \quad \forall\ A$$

$$\sum_I R(A,Z,I) = 1 \quad \forall\ A,Z$$

$$Y(A) = \sum_{Z,I} y(A,Z,I;\vec{x}) \quad \forall\ A$$

$$y = Y(A;\vec{\mu}) \times f(A,Z;\vec{\lambda}) \times R(A,Z,I)$$

Sum yield for a mass chain A
(chain yield can differ by a few percent)

Fractional independent yield

Isomeric yield ratio

Definitions and constraints (cont.)

$$Y(A;\vec{\mu}) \equiv \underbrace{\sum_{i=1,2} \frac{N_i}{\sigma_i\sqrt{2\pi}}\left[e^{-(A-\overline{A}-D_i)^2/2\sigma_i^2} + e^{-(A-\overline{A}+D_i)^2/2\sigma_i^2}\right] + \frac{N_3}{\sigma_3\sqrt{2\pi}} e^{-(A-\overline{A})^2/2\sigma_3^2}}$$

Five Gaussian model

$$\vec{\mu} = \{E, A_f, Z_f, \overline{A}(\nu), N_1, \sigma_1, D_1, N_2, \sigma_2, D_2, \sigma_3\}$$

ν mean number of prompt neutrons

$$N_3 = 2(1 - N_1 - N_2) \quad \Rightarrow \quad \sum_A Y(A;\vec{\mu}) = 2$$

$$f(A,Z;\vec{\lambda}) \equiv \frac{1}{2} F(A,Z)\, N(A)[erf(\frac{Z - Z_p(A) + 1/2}{\sqrt{2}\sigma_Z}) - erf(\frac{Z - Z_p(A) - 1/2}{\sqrt{2}\,\sigma_Z})]$$

$$\vec{\lambda} = \{E, A_f, Z_f, \underbrace{F(A,Z)}, \underbrace{N(A)}, \underbrace{Z_p(A)}, \sigma_Z\}$$

Even-odd effect

Normalization to ensure unity

Unchanged Charge Distribution (UCD)

Covariance matrices (Rebah/Katachura)

$$Cov[y] \equiv \langle \Delta y_c \, \Delta y_{c'} \rangle = \vec{S} \cdot \begin{pmatrix} \langle \Delta Y_c \, \Delta Y_{c'} \rangle & 0 \\ 0 & \langle \Delta f_c \, \Delta f_{c'} \rangle \end{pmatrix} \cdot \vec{S}^T \qquad c = \{A, Z\}$$

$$\vec{S}^T = \left(\frac{\partial y_c}{\partial Y}, \frac{\partial y_c}{\partial f} \right)$$

$$\langle \Delta Y_c \, \Delta Y_{c'} \rangle = \frac{\partial Y_c(\vec{\mu})}{\partial \mu_\ell} \langle \Delta \mu_\ell \, \Delta \mu_m \rangle \frac{\partial Y_{c'}(\vec{\mu})}{\partial \mu_m}$$

$$\langle \Delta f_c \, \Delta f_{c'} \rangle = \frac{\partial f_c(\vec{\lambda})}{\partial \lambda_\ell} \langle \Delta \lambda_\ell \, \Delta \lambda_m \rangle \frac{\partial f_{c'}(\vec{\lambda})}{\partial \lambda_m}$$

Starting from

1) Uncorrelated independent yields
2) Uncorrelated chain mass

$$Cov[y'] = (Cov[y^{-1}] + G^T Cov[Y^{-1}] G)^{-1} \qquad G = \frac{\partial Y_c}{\partial y_{c'}} \equiv \delta_{cc'}$$

$$Var[y'] \equiv \langle \Delta y'_c \, \Delta y'_c \rangle = (\Delta y_c)^2 \left(1 - \frac{(\Delta y_c)^2}{(\Delta Y)^2 + \sum_c (\Delta y_c)^2}\right)$$

$$Cov[y'] \equiv \langle \Delta y'_c \, \Delta y'_{c'} \rangle = -\frac{(\Delta y_c \Delta y_{c'})^2}{(\Delta Y)^2 + \sum_c (\Delta y_c)^2}$$

Definition used also in JENDL Fission Yields Data File 2011 doc (Katakura)

Project summary and timeline

○ Compile uncertainties for nuclear decay data and fission yields

○ Develop methodology to generate covariance matrices

- Deliverable (March 2012) : Interim report documenting models and covariance matrix development

○ Develop ENDF format (file 38?) for independent/cumulative fission product yield covariance matrices (compact format?)

○ Develop perturbed libraries using decay and FPY covariance data and apply the libraries to demonstrate uncertainties for applications to used decay heat, radio toxicity and burn up credit analysis

- Deliverable (September 2012) : Final technical report describing the uncertainty analysis system and data, with quantitative applications to used fuel disposition